

Triethylenetetramine
112-24-3 | DTXSID9023702

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.46e-04 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.83e-01

Confidence level: 2.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Octanol</div> <div>Measured: 4.12e-04</div> <div>Predicted: 6.76e-02</div>	<div>Image not found</div> <div>Nicotine</div> <div>Measured: 5.28e-09</div> <div>Predicted: 3.96e-03</div>	<div>Image not found</div> <div>1-Dodecanethiol</div> <div>Measured: 8.00e-07</div> <div>Predicted: 7.73e-03</div>
<div>Image not found</div> <div>Butyl isocyanate</div> <div>Measured: 2.32e-01</div> <div>Predicted: 17.0</div>	<div>Image not found</div> <div>Diethylenetriamine</div> <div>Measured: 8.19e-03</div> <div>Predicted: 6.12e-02</div>	